

Relating multiway discrepancy and singular values of graphs and contingency tables

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Abstract

The k -way discrepancy $\text{disc}_k(\mathbf{C})$ of a rectangular array \mathbf{C} of nonnegative entries is the minimum of the maxima of the within- and between-cluster discrepancies that can be obtained by simultaneous k -clusterings (proper partitions) of its rows and columns. In Theorem 1, irrespective of the size of \mathbf{C} , we give the following estimate for the k th largest non-trivial singular value of the normalized table: $s_k \leq 9\text{disc}_k(\mathbf{C})(k+2-9k \ln \text{disc}_k(\mathbf{C}))$, provided $\text{disc}_k(\mathbf{C}) < 1$ and $k \leq \text{rank}(\mathbf{C})$. This statement is the converse of Theorem 7 of Bolla [10], and the proof uses some lemmas and ideas of Butler [13], where only the $k=1$ case is treated, in which case our upper bound is the tighter. The result naturally extends to the singular values of the normalized adjacency matrix of a weighted undirected or directed graph.

Keywords: multiway discrepancy; normalized table; singular values; weighted graphs; directed graphs; generalized random graphs.

MSC: 15A18, 05C50

1 Introduction

In many applications, for example when microarrays are analyzed, our data are collected in the form of an $m \times n$ rectangular array $\mathbf{C} = (c_{ij})$ of nonnegative real entries, called contingency table. We assume that \mathbf{C} is non-decomposable, i.e., $\mathbf{C}\mathbf{C}^T$ (when $m \leq n$) or $\mathbf{C}^T\mathbf{C}$ (when $m > n$) is irreducible. Consequently, the row-sums $d_{\text{row},i} = \sum_{j=1}^n c_{ij}$ and column-sums $d_{\text{col},j} = \sum_{i=1}^m c_{ij}$ of \mathbf{C} are strictly positive, and the diagonal matrices $\mathbf{D}_{\text{row}} = \text{diag}(d_{\text{row},1}, \dots, d_{\text{row},m})$ and $\mathbf{D}_{\text{col}} = \text{diag}(d_{\text{col},1}, \dots, d_{\text{col},n})$ are regular. Without loss of generality, we also assume that $\sum_{i=1}^n \sum_{j=1}^m c_{ij} = 1$, since neither our main object, the normalized table

$$\mathbf{C}_{\text{nor}} = \mathbf{D}_{\text{row}}^{-1/2} \mathbf{C} \mathbf{D}_{\text{col}}^{-1/2}, \quad (1)$$

nor the multiway discrepancies to be introduced are affected by the scaling of the entries of \mathbf{C} . It is well known (see e.g., [10]) that the singular values of \mathbf{C}_{nor} are in the $[0,1]$ interval. Enumerated in non-increasing order, they are the real numbers

$$1 = s_0 > s_1 \geq \dots \geq s_{r-1} > s_r = \dots = s_{n-1} = 0,$$

where $r = \text{rank}(\mathbf{C})$. When \mathbf{C} is non-decomposable, 1 is a single singular value, and it is denoted by s_0 , since it belongs to the trivial singular vector pair, which will be disregarded in some further calculations.

Our purpose is to find relations between the k th nontrivial singular value s_k of \mathbf{C}_{nor} and the minimum k -way discrepancy of \mathbf{C} defined herein.

Definition 1 *The multiway discrepancy of the rectangular array \mathbf{C} of nonnegative entries in the proper k -partition R_1, \dots, R_k of its rows and C_1, \dots, C_k of its columns is*

$$\text{disc}(\mathbf{C}; R_1, \dots, R_k, C_1, \dots, C_k) = \max_{\substack{1 \leq a \leq b \leq k \\ X \subset R_a, Y \subset C_b}} \frac{|c(X, Y) - \rho(R_a, C_b) \text{Vol}(X) \text{Vol}(Y)|}{\sqrt{\text{Vol}(X) \text{Vol}(Y)}}, \quad (2)$$

where $c(X, Y) = \sum_{i \in X} \sum_{j \in Y} c_{ij}$ is the cut between $X \subset R_a$ and $Y \subset C_b$, $\text{Vol}(X) = \sum_{i \in X} d_{\text{row}, i}$ is the volume of the row-subset X , $\text{Vol}(Y) = \sum_{j \in Y} d_{\text{col}, j}$ is the volume of the column-subset Y , whereas $\rho(R_a, C_b) = \frac{c(R_a, C_b)}{\text{Vol}(R_a) \text{Vol}(C_b)}$ denotes the relative density between R_a and C_b . The minimum k -way discrepancy of \mathbf{C} itself is

$$\text{disc}_k(\mathbf{C}) = \min_{\substack{R_1, \dots, R_k \\ C_1, \dots, C_k}} \text{disc}(\mathbf{C}; R_1, \dots, R_k, C_1, \dots, C_k).$$

In Section 4, I will extend this notion to an edge-weighted graph G and denote it by $\text{disc}_k(G)$. In that setup, \mathbf{C} plays the role of the edge-weight matrix (symmetric in the undirected; quadratic, but usually not symmetric in the directed case; and it is the adjacency matrix if G is a simple graph when the eigenvalues of the normalized adjacency matrix enter into the estimates, in their decreasing absolute values).

Note that $\text{disc}(\mathbf{C}; R_1, \dots, R_k, C_1, \dots, C_k)$ is the smallest α such that for every R_a, C_b pair and for every $X \subset R_a, Y \subset C_b$,

$$|c(X, Y) - \rho(R_a, C_b) \text{Vol}(X) \text{Vol}(Y)| \leq \alpha \sqrt{\text{Vol}(X) \text{Vol}(Y)} \quad (3)$$

holds. Hence, in the k -partitions of the rows and columns, giving the minimum k -way discrepancy (say, α^*) of \mathbf{C} , every R_a, C_b pair is α^* -regular in terms of the volumes, and α^* is the smallest possible discrepancy that can be attained with proper k -partitions. It resembles the notion of ϵ -regular pairs in the Szemerédi regularity lemma [26], albeit with given number of vertex-clusters, which are usually not equitable; further, with volumes, instead of cardinalities.

Historically, the notion of discrepancy together with the expander mixing lemma was introduced for simple, regular graphs, see e.g., Alon, Spencer, Hoory, Linial, Wigderson [2, 21], and extended to Hermitian matrices in Bollobás, Nikiforov [11]. In Chung, Graham, Wilson [15], the authors use the term quasirandom for simple graphs that satisfy any of some equivalent properties, some of them closely related to discrepancy and eigenvalue separation. Chung and Graham [16] prove that for simple graphs ‘small’ discrepancy $\text{disc}(G)$ (with our notation, $\text{disc}_1(G)$) is caused by eigenvalue ‘separation’: the second largest singular value (which is also the second largest absolute value eigenvalue), s_1 , of the normalized adjacency matrix is ‘small’, i.e., separated from the trivial singular value $s_0 = 1$, which is the edge of the spectrum. More exactly, they prove $\text{disc}(G) \leq s_1$, hence giving some kind of generalization of the expander mixing lemma for *irregular* graphs.

In the other direction, for Hermitian matrices, Bollobás and Nikiforov [11] estimate the second largest singular value of an $n \times n$ Hermitian matrix \mathbf{A} by $C \text{disc}(\mathbf{A}) \log n$, and show that this is best possible up to a multiplicative constant. Bilu and Linial [4] prove the converse of the expander mixing lemma for simple regular graphs, but their key Lemma 3.3, producing this statement,

goes beyond regular graphs. In Alon et al. [3], the authors relax the notion of eigenvalue separation to essential eigenvalue separation (by introducing a parameter for it, and requiring the separation only for the eigenvalues of a relatively large part of the graph). Then they prove relations between the constants of this kind of eigenvalue separation and discrepancy.

For a general rectangular array \mathbf{C} of nonnegative entries, Butler [13] proves the following forward and backward statement in the $k = 1$ case:

$$\text{disc}(\mathbf{C}) \leq s_1 \leq 150\text{disc}(\mathbf{C})(1 - 8 \ln \text{disc}(\mathbf{C})), \quad (4)$$

where $\text{disc}(\mathbf{C})$ is our $\text{disc}_1(\mathbf{C})$ and, with our notation, s_1 is the largest nontrivial singular value of \mathbf{C}_D (he denotes it with σ_2). Since $s_1 < 1$, the upper estimate makes sense for very small discrepancy, in particular, for $\text{disc}(\mathbf{C}) \leq 8.868 \times 10^{-5}$. The lower estimate further generalizes the expander mixing lemma to rectangular matrices, but it can be proved with the same tools as in the quadratic case (see Proposition 2 in Section 4).

So far, the overall discrepancy has been considered in the sense, that $\text{disc}(\mathbf{C})$ or $\text{disc}(G)$ measures the largest possible deviation between the actual and expected connectedness of arbitrary (sometimes disjoint) subsets X, Y , where under expected the hypothesis of independence is understood (which corresponds to the rank 1 approximation). Note that in [13, 14], $\text{disc}_t(G)$ (or $\text{AltDisc}_t(G)$ for alternating walks in directed graphs) is also introduced, which measures the minimum possible deviation between the actual and expected number of walks of length t between the vertex-subsets. Similar notion appears in [16], and other notions of discrepancy are also introduced in [17]; for example, the skew-discrepancy for directed graphs. Notwithstanding, these papers consider variants of the overall discrepancy, which corresponds to the one-cluster situation.

My purpose is, in the multicluster scenario, to find similar relations between the minimum k -way discrepancy and the SVD of the normalized matrix, for given k . In one direction, in Section 2, I will prove the following.

Theorem 1 *For every non-decomposable contingency table \mathbf{C} and integer $1 \leq k \leq \text{rank}(\mathbf{C})$,*

$$s_k \leq 9\text{disc}_k(\mathbf{C})(k + 2 - 9k \ln \text{disc}_k(\mathbf{C})),$$

provided $\text{disc}_k(\mathbf{C}) < 1$, where s_k is the k th largest non-trivial singular value of the normalized table \mathbf{C}_{nor} introduced in (1).

Note that $\text{disc}_k(\mathbf{C}) = 0$ only if \mathbf{C} has a block structure with k row- and column-blocks, in which case $s_k = 0$ also holds. Likewise, $\text{disc}_k(\mathbf{C}) < 1$ is not a peculiar requirement, since in view of $s_k < 1$, the upper bound of the theorem has relevance only for $\text{disc}_k(\mathbf{C})$ much smaller than 1; for example, for $\text{disc}_1(\mathbf{C}) \leq 1.866 \times 10^{-3}$, $\text{disc}_2(\mathbf{C}) \leq 8.459 \times 10^{-4}$, $\text{disc}_3(\mathbf{C}) \leq 5.329 \times 10^{-4}$, etc.

In the other direction, in Theorem 7 of [10], I showed that (under some balancing conditions on the margins and cluster sizes) a bit modified version of this k -way discrepancy is $O(\sqrt{2k}S_k + s_k)$, where S_k is the sum of the squareroots of the k -variances of the optimal row- and column-representatives (they depend on the normalized singular vectors corresponding to s_1, \dots, s_{k-1}). In fact, S_k the smaller, the larger the gap between s_k and s_{k-1} is. I will better explain

this notion in Section 3. There I will also illustrate that $S_k = 0$ holds in many special cases, and consequently, my upper estimate for the k -way discrepancy boils down to Bs_k with some absolute constant B . For example, in the simple graph case, when $k = 2$ and our graph is bipartite, biregular, the discrepancy between the two independent vertex-sets is estimated from above with Bs_2 by my result, and, up to a constant factor, this is the same as the estimate proved in Evra et al. [18]. In Section 3, I will also mention some spectral relations to the weak Szemerédi regularity lemma [12, 19, 20, 25].

2 Proof of Theorem 1

Before proving the theorem, I encounter some lemmas of others that I will use, possibly with some modifications.

Lemma 3 of Bollobás and Nikiforov [11] is the key to prove their main result. This lemma states that to every $0 < \varepsilon < 1$ and vector $\mathbf{x} \in \mathbb{C}^n$, $\|\mathbf{x}\| = 1$, there exists a vector $\mathbf{y} \in \mathbb{C}^n$ such that its coordinates take no more than $\lceil \frac{8\pi}{\varepsilon} \rceil \lceil \frac{4}{\varepsilon} \log \frac{2n}{\varepsilon} \rceil$ distinct values and $\|\mathbf{x} - \mathbf{y}\| \leq \varepsilon$. This is why $\log n$ appears in their estimate for the second largest singular value of an $n \times n$ Hermitian matrix. Since I do not want to appear the log-sizes in my estimate in the miniature world of $[0, 1]$, I will rather use the construction of the following lemma, which is indeed a consequence of Lemma 3 of [11].

Lemma 1 (Lemma 3 of Butler [13]) *To any vector $\mathbf{x} \in \mathbb{C}^n$, $\|\mathbf{x}\| = 1$ and diagonal matrix \mathbf{D} of positive real diagonal entries, one can construct a step-vector $\mathbf{y} \in \mathbb{C}^n$ such that $\|\mathbf{x} - \mathbf{D}\mathbf{y}\| \leq \frac{1}{3}$, $\|\mathbf{D}\mathbf{y}\| \leq 1$, and the nonzero entries of \mathbf{y} are of the form $(\frac{4}{5})^j e^{\frac{\ell}{29} 2\pi i}$ with appropriate integers j and ℓ ($0 \leq \ell \leq 28$).*

Note that starting with an \mathbf{x} of real coordinates, we do not need all the 29 values of ℓ , only two of them will show up, as it follows from a better understanding of the construction of [13]. In fact, by the idea of [11], j 's come from dividing the coordinates of $\mathbf{D}^{-1}\mathbf{x}/\|\mathbf{D}^{-1}\mathbf{x}\|$ in decreasing absolute values into groups, where the cut-points are powers of $\frac{4}{5}$. With the notation $\mathbf{x} = (x_s)_{s=1}^n$, if x_s is in the j -th group, then the corresponding coordinate of the approximating complex vector $\mathbf{y} = (y_s)_{s=1}^n$ is as follows. If $x_s = 0$, then $y_s = 0$, otherwise $y_s = (\frac{4}{5})^j e^{(\lfloor \frac{29\theta}{2\pi} \rfloor / 29) 2\pi i}$, where θ is the argument of x_s , $0 \leq \theta < 2\pi$, and therefore, $\ell = \lfloor \frac{29\theta}{2\pi} \rfloor$ is an integer between 0 and 28. However, when the coordinates of \mathbf{x} are real numbers, then only the values 0 and 14 of ℓ can occur, since θ can take only one of the values 0 or π , depending on whether x_s is positive or negative. We will intensively use this observation in our proof.

Lemma 2 (Lemma 4 of Butler [13]) *Let \mathbf{M} be a matrix with largest singular value σ and corresponding unit-norm singular vector pair \mathbf{v}, \mathbf{u} . If \mathbf{x} and \mathbf{y} are vectors such that $\|\mathbf{x}\| \leq 1$, $\|\mathbf{y}\| \leq 1$, $\|\mathbf{v} - \mathbf{x}\| \leq \frac{1}{3}$, $\|\mathbf{u} - \mathbf{y}\| \leq \frac{1}{3}$, then $\sigma \leq \frac{9}{2} \langle \mathbf{x}, \mathbf{M}\mathbf{y} \rangle$.*

Note that, in our case, \mathbf{M} is a real matrix and so, \mathbf{v}, \mathbf{u} have real coordinates; still, the approximating (step-vectors) \mathbf{x}, \mathbf{y} may have complex coordinates, and so, $\langle \cdot, \cdot \rangle$ denotes the (possibly complex) inner product. Note that in the possession of real (column) vectors \mathbf{x}, \mathbf{y} and matrix \mathbf{M} , $\langle \cdot, \cdot \rangle$ can be written in terms of matrix-vector multiplications with transpositions: $\langle \mathbf{x}, \mathbf{M}\mathbf{y} \rangle = \mathbf{x}^T \mathbf{M}\mathbf{y}$.

Proof (of the main theorem). Assume that $\alpha := \text{disc}_k(\mathbf{C}) < 1$ and it is attained with the proper k -partition R_1, \dots, R_k of the rows and C_1, \dots, C_k of the columns of \mathbf{C} ; i.e., for every R_a, C_b pair and $X \subset R_a, Y \subset C_b$ we have

$$|c(X, Y) - \rho(R_a, C_b) \text{Vol}(X) \text{Vol}(Y)| \leq \alpha \sqrt{\text{Vol}(X) \text{Vol}(Y)}. \quad (5)$$

Our purpose is to put Inequality (5) in matrix form by using indicator vectors and introducing the $m \times n$ auxiliary matrix

$$\mathbf{F} = \mathbf{C} - \mathbf{D}_{\text{row}} \mathbf{R} \mathbf{D}_{\text{col}}, \quad (6)$$

where $\mathbf{R} = (\rho(R_a, C_b))$ is the $m \times n$ block-matrix of $k \times k$ blocks with entries equal to $\rho(R_a, C_b)$ over the block $R_a \times C_b$. With the indicator vectors $\mathbf{1}_X$ and $\mathbf{1}_Y$ of $X \subset R_a$ and $Y \subset C_b$, Inequality (5) has the following equivalent form:

$$|\langle \mathbf{1}_X, \mathbf{F} \mathbf{1}_Y \rangle| \leq \alpha \sqrt{\langle \mathbf{1}_X, \mathbf{C} \mathbf{1}_n \rangle \langle \mathbf{1}_m, \mathbf{C} \mathbf{1}_Y \rangle} \quad (7)$$

where $\mathbf{1}_n$ denotes the all 1's vector of size n and $\langle \cdot, \cdot \rangle$ denotes the (possibly complex) inner product. Note that in the possession of real (column) vectors and matrices, $\langle \cdot, \cdot \rangle$ can be written in terms of matrix-vector multiplications with transpositions; for example, $\langle \mathbf{1}_X, \mathbf{F} \mathbf{1}_Y \rangle = \mathbf{1}_X^T \mathbf{F} \mathbf{1}_Y$. At the same time, Equation (6) yields

$$\mathbf{D}_{\text{row}}^{-1/2} \mathbf{F} \mathbf{D}_{\text{col}}^{-1/2} = \mathbf{D}_{\text{row}}^{-1/2} \mathbf{C} \mathbf{D}_{\text{col}}^{-1/2} - \mathbf{D}_{\text{row}}^{1/2} \mathbf{R} \mathbf{D}_{\text{col}}^{1/2} = \mathbf{C}_{\text{nor}} - \mathbf{D}_{\text{row}}^{1/2} \mathbf{R} \mathbf{D}_{\text{col}}^{1/2}.$$

Since the rank of the matrix $\mathbf{D}_{\text{row}}^{1/2} \mathbf{R} \mathbf{D}_{\text{col}}^{1/2}$ is at most k , by Theorem 3 of Thompson¹ [27], describing the effect of rank k perturbations for the singular values, we obtain the following upper estimate for s_k , that is the $(k+1)$ th largest (including the trivial 1) singular value of \mathbf{C}_{nor} :

$$s_k \leq s_{\max}(\mathbf{D}_{\text{row}}^{-1/2} \mathbf{F} \mathbf{D}_{\text{col}}^{-1/2}) = \|\mathbf{D}_{\text{row}}^{-1/2} \mathbf{F} \mathbf{D}_{\text{col}}^{-1/2}\|,$$

where $\|\cdot\|$ denotes the spectral norm.

Let $\mathbf{v} \in \mathbb{R}^m$ be the left and $\mathbf{u} \in \mathbb{R}^n$ be the right unit-norm singular vector corresponding to the maximal singular value of $\mathbf{D}_{\text{row}}^{-1/2} \mathbf{F} \mathbf{D}_{\text{col}}^{-1/2}$, i.e.,

$$|\langle \mathbf{v}, (\mathbf{D}_{\text{row}}^{-1/2} \mathbf{F} \mathbf{D}_{\text{col}}^{-1/2}) \mathbf{u} \rangle| = \|\mathbf{D}_{\text{row}}^{-1/2} \mathbf{F} \mathbf{D}_{\text{col}}^{-1/2}\|.$$

In view of Lemma 1, there are stepwise constant vectors $\mathbf{x} \in \mathbb{C}^m$ and $\mathbf{y} \in \mathbb{C}^n$ such that $\|\mathbf{v} - \mathbf{D}_{\text{row}}^{1/2} \mathbf{x}\| \leq \frac{1}{3}$ and $\|\mathbf{u} - \mathbf{D}_{\text{col}}^{1/2} \mathbf{y}\| \leq \frac{1}{3}$; further, $\|\mathbf{D}_{\text{row}}^{1/2} \mathbf{x}\| \leq 1$ and $\|\mathbf{D}_{\text{col}}^{1/2} \mathbf{y}\| \leq 1$. Then Lemma 2 yields

$$\|\mathbf{D}_{\text{row}}^{-1/2} \mathbf{F} \mathbf{D}_{\text{col}}^{-1/2}\| \leq \frac{9}{2} \left| \langle (\mathbf{D}_{\text{row}}^{1/2} \mathbf{x}), (\mathbf{D}_{\text{row}}^{-1/2} \mathbf{F} \mathbf{D}_{\text{col}}^{-1/2}) (\mathbf{D}_{\text{col}}^{1/2} \mathbf{y}) \rangle \right| = \frac{9}{2} |\langle \mathbf{x}, \mathbf{F} \mathbf{y} \rangle|.$$

Now we will use the construction in the proof of the Lemma 3 [13] in the special case when the vectors $\mathbf{v} = (v_s)_{s=1}^m$ and $\mathbf{u} = (u_s)_{s=1}^n$, to be approximated, have

¹Actually, Thompson stated the theorem for square matrices, but in the possession of a rectangular one, we can supplement it with zero rows or columns to make it quadratic; further, the nonzero singular values of the so obtained square matrix are the same as those of the rectangular, supplemented with additional zero singular values that will not alter the shifted interlacing facts.

real coordinates. Therefore, only the following three types of coordinates of the approximating complex vectors $\mathbf{x} = (x_s)_{s=1}^m$ and $\mathbf{y} = (y_s)_{s=1}^n$ will appear. If $v_s = 0$, then $x_s = 0$ too; if $v_s > 0$, then $x_s = (\frac{4}{5})^j$ with some integer j ; if $v_s < 0$, then $x_s = (\frac{4}{5})^j e^{\frac{28}{29}\pi i}$ with some integer j . Likewise, if $u_s = 0$, then $y_s = 0$ too; if $u_s > 0$, then $y_s = (\frac{4}{5})^\ell$ with some integer ℓ ; if $u_s < 0$, then $y_s = (\frac{4}{5})^\ell e^{\frac{28}{29}\pi i}$ with some integer ℓ . With these observations, the step-vectors \mathbf{x} and \mathbf{y} can be written as the following finite sums with respect to the integers j and ℓ :

$$\mathbf{x} = \sum_j \left(\frac{4}{5}\right)^j \mathbf{x}^{(j)}, \quad \mathbf{x}^{(j)} = \sum_{a=1}^k (\mathbf{1}_{\mathcal{X}_{ja1}} + e^{\frac{28}{29}\pi i} \mathbf{1}_{\mathcal{X}_{ja2}}), \quad \text{where}$$

$$\mathcal{X}_{ja1} = \{s : x_s = (\frac{4}{5})^j, s \in R_a\} \quad \text{and} \quad \mathcal{X}_{ja2} = \{s : x_s = (\frac{4}{5})^j e^{\frac{28}{29}\pi i}, s \in R_a\};$$

likewise,

$$\mathbf{y} = \sum_\ell \left(\frac{4}{5}\right)^\ell \mathbf{y}^{(\ell)}, \quad \mathbf{y}^{(\ell)} = \sum_{b=1}^k (\mathbf{1}_{\mathcal{Y}_{\ell b1}} + e^{\frac{28}{29}\pi i} \mathbf{1}_{\mathcal{Y}_{\ell b2}}), \quad \text{where}$$

$$\mathcal{Y}_{\ell b1} = \{s : y_s = (\frac{4}{5})^\ell, s \in C_b\} \quad \text{and} \quad \mathcal{Y}_{\ell b2} = \{s : y_s = (\frac{4}{5})^\ell e^{\frac{28}{29}\pi i}, s \in C_b\}.$$

Then

$$\begin{aligned} |\langle \mathbf{x}^{(j)}, \mathbf{F}\mathbf{y}^{(\ell)} \rangle| &\leq \sum_{a=1}^k \sum_{b=1}^k \sum_{p=1}^2 \sum_{q=1}^2 |\langle \mathbf{1}_{\mathcal{X}_{ja p}}, \mathbf{F}\mathbf{1}_{\mathcal{Y}_{\ell b q}} \rangle| \\ &\stackrel{(7)}{\leq} \sum_{a=1}^k \sum_{b=1}^k \sum_{p=1}^2 \sum_{q=1}^2 \alpha \sqrt{\langle \mathbf{1}_{\mathcal{X}_{ja p}}, \mathbf{C}\mathbf{1}_n \rangle \langle \mathbf{1}_m, \mathbf{C}\mathbf{1}_{\mathcal{Y}_{\ell b q}} \rangle} \\ &\leq \alpha 2k \sqrt{\sum_{a=1}^k \sum_{b=1}^k \sum_{p=1}^2 \sum_{q=1}^2 \langle \mathbf{1}_{\mathcal{X}_{ja p}}, \mathbf{C}\mathbf{1}_n \rangle \langle \mathbf{1}_m, \mathbf{C}\mathbf{1}_{\mathcal{Y}_{\ell b q}} \rangle} \quad (8) \\ &= 2k\alpha \sqrt{\langle \sum_{a=1}^k \sum_{p=1}^2 \mathbf{1}_{\mathcal{X}_{ja p}}, \mathbf{C}\mathbf{1}_n \rangle \langle \mathbf{1}_m, \mathbf{C} \sum_{b=1}^k \sum_{q=1}^2 \mathbf{1}_{\mathcal{Y}_{\ell b q}} \rangle} \\ &= 2k\alpha \sqrt{\langle |\mathbf{x}^{(j)}|, \mathbf{C}\mathbf{1}_n \rangle \langle \mathbf{1}_m, \mathbf{C}|\mathbf{y}^{(\ell)}| \rangle}, \end{aligned}$$

where in the first inequality we used that $|e^{\frac{28}{29}\pi i}| = 1$, in the second one we used (7), while in the last one, the Cauchy-Schwarz inequality with $4k^2$ terms. We also introduced the notation $|\mathbf{z}| = (|z_s|)_{s=1}^n$ for the real vector, the coordinates of which are the absolute values of the corresponding coordinates of the (possibly complex) vector \mathbf{z} . In the same spirit, let $|\mathbf{M}|$ denote the matrix whose entries are the absolute values of the corresponding entries of \mathbf{M} (we will use this only for real matrices). With this formalism, this is the right moment to prove the following inequalities that will be used soon to finish the proof:

$$\sum_\ell |\langle \mathbf{x}^{(j)}, \mathbf{F}\mathbf{y}^{(\ell)} \rangle| \leq 2\langle |\mathbf{x}^{(j)}|, \mathbf{C}\mathbf{1}_n \rangle, \quad \sum_j |\langle \mathbf{x}^{(j)}, \mathbf{F}\mathbf{y}^{(\ell)} \rangle| \leq 2\langle \mathbf{1}_m, \mathbf{C}|\mathbf{y}^{(\ell)}| \rangle. \quad (9)$$

Since the two inequalities are of the same flavor, it suffices to prove only the first one. Note that it is here, where we use the exact definition of \mathbf{F} as follows.

$$\begin{aligned} \sum_{\ell} |\langle \mathbf{x}^{(j)}, \mathbf{F}\mathbf{y}^{(\ell)} \rangle| &\leq \langle |\mathbf{x}^{(j)}|, |\mathbf{F}| \sum_{\ell} |\mathbf{y}^{(\ell)}| \rangle \\ &\leq \langle |\mathbf{x}^{(j)}|, (\mathbf{C} + \mathbf{D}_{row} \mathbf{R} \mathbf{D}_{col}) \mathbf{1}_n \rangle = 2 \langle |\mathbf{x}^{(j)}|, \mathbf{C} \mathbf{1}_n \rangle \end{aligned}$$

because $|\mathbf{y}^{(\ell)}|$ is a 0-1 vector and $\mathbf{C} + \mathbf{D}_{row} \mathbf{R} \mathbf{D}_{col}$ is a (real) matrix of nonnegative entries. We also used that the i th coordinate of the vector $(\mathbf{C} + \mathbf{D}_{row} \mathbf{R} \mathbf{D}_{col}) \mathbf{1}_n$ for $i \in R_a$ is

$$d_{row,i} \left(1 + \sum_{b=1}^k \rho(R_a, C_b) \text{Vol}(C_b) \right) = 2d_{row,i}$$

(here we utilized that the sum of the entries of \mathbf{C} is 1), and therefore,

$$(\mathbf{C} + \mathbf{D}_{row} \mathbf{R} \mathbf{D}_{col}) \mathbf{1}_n = 2\mathbf{C} \mathbf{1}_n.$$

Finally, we will finish the proof with similar calculations as in [13]. Let us further estimate

$$\langle \mathbf{x}, \mathbf{F}\mathbf{y} \rangle = \sum_j \sum_{\ell} \langle (\frac{4}{5})^j \mathbf{x}^{(j)}, \mathbf{F}(\frac{4}{5})^{\ell} \mathbf{y}^{(\ell)} \rangle.$$

Put $\gamma := \log_{4/5} \alpha$; in view of $\alpha < 1$, $\gamma > 0$ holds. Then we divide the above summation into three parts as follows.

$$\begin{aligned} |\langle \mathbf{x}, \mathbf{F}\mathbf{y} \rangle| &\leq \sum_j \sum_{\ell} (\frac{4}{5})^{j+\ell} |\langle \mathbf{x}^{(j)}, \mathbf{F}\mathbf{y}^{(\ell)} \rangle| \\ &= \sum_{\substack{|j-\ell| \leq \gamma \\ \text{(a)}}} (\frac{4}{5})^{j+\ell} |\langle \mathbf{x}^{(j)}, \mathbf{F}\mathbf{y}^{(\ell)} \rangle| + \sum_{\substack{j-\ell > \gamma \\ \text{(b)}}} (\frac{4}{5})^{j+\ell} |\langle \mathbf{x}^{(j)}, \mathbf{F}\mathbf{y}^{(\ell)} \rangle| + \sum_{\substack{j-\ell < -\gamma \\ \text{(c)}}} (\frac{4}{5})^{j+\ell} |\langle \mathbf{x}^{(j)}, \mathbf{F}\mathbf{y}^{(\ell)} \rangle|. \end{aligned}$$

The three terms are estimated separately. Term (a) can be bounded from above as follows:

$$\begin{aligned} \sum_{|j-\ell| \leq \gamma} (\frac{4}{5})^{j+\ell} |\langle \mathbf{x}^{(j)}, \mathbf{F}\mathbf{y}^{(\ell)} \rangle| &\stackrel{(8)}{\leq} 2k\alpha \sum_{|j-\ell| \leq \gamma} \sqrt{(\frac{4}{5})^{2j} \langle |\mathbf{x}^{(j)}|, \mathbf{C} \mathbf{1}_n \rangle (\frac{4}{5})^{2\ell} \langle \mathbf{1}_m, \mathbf{C} |\mathbf{y}^{(\ell)}| \rangle} \\ &\stackrel{(*)}{\leq} k\alpha \sum_{|j-\ell| \leq \gamma} \left[(\frac{4}{5})^{2j} \langle |\mathbf{x}^{(j)}|, \mathbf{C} \mathbf{1}_n \rangle + (\frac{4}{5})^{2\ell} \langle \mathbf{1}_m, \mathbf{C} |\mathbf{y}^{(\ell)}| \rangle \right] \\ &\stackrel{(**)}{\leq} k\alpha(2\gamma + 1) \left[\sum_j (\frac{4}{5})^{2j} \langle |\mathbf{x}^{(j)}|, \mathbf{C} \mathbf{1}_n \rangle + \sum_{\ell} (\frac{4}{5})^{2\ell} \langle \mathbf{1}_m, \mathbf{C} |\mathbf{y}^{(\ell)}| \rangle \right] \\ &\stackrel{(***)}{\leq} 2k\alpha(2\gamma + 1), \end{aligned}$$

where in the first inequality, the estimate of (8) and in (*), the geometric-arithmetic mean inequality were used; (**) comes from the fact that in summation (a), for fixed j or ℓ , any term can show up at most $2\gamma + 1$ times, and (***)

is due to the easy observation that

$$\sum_j \left(\frac{4}{5}\right)^{2j} \langle |\mathbf{x}^{(j)}|, \mathbf{C}\mathbf{1}_n \rangle = \|\mathbf{D}_{row}^{1/2} \mathbf{x}\|^2 \leq 1, \quad \sum_\ell \left(\frac{4}{5}\right)^{2\ell} \langle \mathbf{1}_m, \mathbf{C}|\mathbf{y}^{(\ell)} \rangle = \|\mathbf{D}_{col}^{1/2} \mathbf{y}\|^2 \leq 1. \quad (10)$$

Terms (b) and (c) are of similar appearance (the role of j and ℓ is symmetric in them), therefore, we will estimate only (b). Here $j - \ell > \gamma$, yielding $j + \ell > 2\ell + \gamma$. Therefore,

$$\begin{aligned} \sum_{j-\ell > \gamma} \left(\frac{4}{5}\right)^{j+\ell} |\langle \mathbf{x}^{(j)}, \mathbf{F}\mathbf{y}^{(\ell)} \rangle| &\leq \sum_\ell \left(\frac{4}{5}\right)^{2\ell+\gamma} \sum_j |\langle \mathbf{x}^{(j)}, \mathbf{F}\mathbf{y}^{(\ell)} \rangle| \\ &\stackrel{(9)}{\leq} \sum_\ell \left(\frac{4}{5}\right)^{2\ell+\gamma} 2 \langle \mathbf{1}_m, \mathbf{C}|\mathbf{y}^{(\ell)} \rangle \\ &= 2 \left(\frac{4}{5}\right)^\gamma \sum_\ell \left(\frac{4}{5}\right)^{2\ell} \langle \mathbf{1}_m, \mathbf{C}|\mathbf{y}^{(\ell)} \rangle \stackrel{(10)}{\leq} 2 \left(\frac{4}{5}\right)^\gamma. \end{aligned}$$

where, in the second and third inequalities, (9) and (10) were used. Consequently, (c) can also be estimated from above with $2\left(\frac{4}{5}\right)^\gamma$.

Collecting the so obtained estimates together, we get

$$\begin{aligned} s_k &\leq \frac{9}{2} |\langle \mathbf{x}, \mathbf{F}\mathbf{y} \rangle| \leq \frac{9}{2} \left[2k\alpha(2\gamma + 1) + 4\left(\frac{4}{5}\right)^\gamma \right] = 9\alpha \left[2k \frac{\ln \alpha}{\ln \frac{4}{5}} + k + 2 \right] \\ &\leq 9\alpha [2k(-4.5) \ln \alpha + k + 2] = 9\alpha(k + 2 - 9k \ln \alpha), \end{aligned}$$

that was to be proved. For $k = 1$, our upper bound is tighter than that of (4).

3 Some weaker results

Now about our first attempts to prove something like Theorem 1, because they may be informative for the reader.

- First we wanted to use Lemma 3 of Bollobás and Nikiforov [11], since, in addition, it specifies the number of distinct coordinates of the approximating step-vector. This lemma states that to every $0 < \varepsilon < 1$ and vector $\mathbf{x} \in \mathbf{C}^n$, $\|\mathbf{x}\| = 1$, there is a vector $\mathbf{y} \in \mathbf{C}^n$ such that its coordinates take no more than

$$\left\lceil \frac{8\pi}{\varepsilon} \right\rceil \left\lceil \frac{4}{\varepsilon} \log \frac{2n}{\varepsilon} \right\rceil \quad (11)$$

values and $\|\mathbf{x} - \mathbf{y}\| \leq \varepsilon$.

Note that this lemma implies Lemma 3 of Butler [13], which states that to any unit-norm vector $\mathbf{x} \in \mathbf{C}^n$ and diagonal matrix \mathbf{D} of positive diagonal entries, one can construct a step-vector $\mathbf{y} \in \mathbf{C}^n$ such that $\|\mathbf{x} - \mathbf{D}\mathbf{y}\| \leq \varepsilon$ and $\|\mathbf{D}\mathbf{y}\| \leq 1$. Even the construction of the two lemmas are similar.

In our case, $\mathbf{x} \in \mathbb{R}^n$ and we need $1/3$ precision. Given the diagonal matrix \mathbf{D} of positive diagonal entries, we will now construct a step-vector \mathbf{y} of complex entries such that $\|\mathbf{x} - \mathbf{D}\mathbf{y}\| \leq 1/3$, by merely using Lemma 3 of [11]. First set $f := \|\mathbf{D}^{-1}\mathbf{x}\|$ and $d := \|\mathbf{D}\| = \max_i d_i$. Then, by [11],

to the unit-norm vector $\mathbf{D}^{-1}\mathbf{x}/f$ and to $0 < \varepsilon < 1$ there is a step-vector $\mathbf{y} \in \mathbb{C}^n$, with the same number of different coordinates as in (11), such that

$$\left\| \frac{\mathbf{D}^{-1}\mathbf{x}}{f} - \mathbf{y} \right\| \leq \varepsilon.$$

The step-vector $\mathbf{z} = f\mathbf{y} \in \mathbb{C}^n$, with the same number of different coordinates as in \mathbf{y} , will do for us, since with an appropriate ε we can reach that $\|\mathbf{x} - \mathbf{D}\mathbf{z}\| \leq \frac{1}{3}$. Indeed,

$$\varepsilon \geq \left\| \frac{\mathbf{D}^{-1}\mathbf{x}}{f} - \mathbf{y} \right\| = \frac{1}{f} \|\mathbf{D}^{-1}(\mathbf{x} - \mathbf{D}\mathbf{z})\| \geq \frac{1}{f} \min_i \frac{1}{d_i} \|\mathbf{x} - \mathbf{D}\mathbf{z}\| = \frac{1}{fd} \|\mathbf{x} - \mathbf{D}\mathbf{z}\|.$$

Therefore,

$$\|\mathbf{x} - \mathbf{D}\mathbf{z}\| \leq fd\varepsilon = \frac{1}{3}$$

holds with $\varepsilon = \frac{1}{3fd}$ that cannot exceed $\frac{1}{3}$, since $fd \geq 1$. This can be seen from the following argument:

$$1 = \|\mathbf{x}\| = \|\mathbf{D}\mathbf{D}^{-1}\mathbf{x}\| \leq \|\mathbf{D}\| \cdot \|\mathbf{D}^{-1}\mathbf{x}\| = df.$$

Eventually, by the construction of [11], $|y_j| \leq \frac{|x_j|}{d_j f}$, $j = 1, \dots, n$. Therefore, $|z_j| = f|y_j| \leq \frac{|x_j|}{d_j}$, and $|d_j z_j| \leq |x_j|$, $\forall j$. Consequently, $\|\mathbf{D}\mathbf{z}\| \leq \|\mathbf{x}\| = 1$.

The main implication of this fact is that the maximal number of distinct coordinates of the step-vector in Lemma 3 of [13] is also of order $\log n$, and we wanted to make use of this fact in the first attempts of the proof of some backward statement. For this purpose, we managed to prove the following lemma, inspired by Lemma 4 of [11], though, in a more general setup. We will give the proof too, since it may be of interest for its own right.

Lemma 3 *Let \mathbf{C} be an $m \times n$ matrix of nonnegative real entries and let the rows and columns have positive real weights $d_{r,i}$'s and $d_{c,j}$'s (independently of the entries of \mathbf{C}), which are collected in the main diagonals of the $m \times m$ and $n \times n$ diagonal matrices \mathbf{D}_r and \mathbf{D}_c , respectively. Let R_1, \dots, R_k and C_1, \dots, C_ℓ be proper partitions of the rows and columns; further, $\mathbf{x} \in \mathbb{C}^m$ and $\mathbf{y} \in \mathbb{C}^n$ be stepwise constant vectors having equal coordinates over the index sets corresponding to the partition members of R_1, \dots, R_k and C_1, \dots, C_ℓ , respectively. The $k \times \ell$ real matrix $\mathbf{C}' = (c'_{ab})$ is defined by*

$$c'_{ab} := \frac{c(R_a, C_b)}{\sqrt{\text{VOL}(R_a)\text{VOL}(C_b)}}, \quad a = 1, \dots, k; b = 1, \dots, \ell,$$

where $c(R_a, C_b)$ is the usual cut of \mathbf{C} between R_a and C_b , whereas $\text{VOL}(R_a) = \sum_{i \in R_a} d_{r,i}$ and $\text{VOL}(C_b) = \sum_{j \in C_b} d_{c,j}$. Then

$$|\langle \mathbf{x}, \mathbf{C}\mathbf{y} \rangle| \leq \|\mathbf{C}'\| \cdot \|\mathbf{D}_r^{1/2}\mathbf{x}\| \cdot \|\mathbf{D}_c^{1/2}\mathbf{y}\|,$$

where $\|\mathbf{C}'\|$ denotes the spectral norm, that is the largest singular value of the real matrix \mathbf{C}' , and the squared norm of a complex vector is the sum of the squares of the absolute values of its coordinates.

Note that here the row- and column-weights have nothing to do with the entries of \mathbf{C} , and the volumes are usually not the ones defined in Section 1; this is why they are denoted by VOL instead of Vol.

Proof of Lemma 3 For the distinct coordinates of \mathbf{x} and \mathbf{y} we introduce

$$x_i := \frac{x'_a}{\sqrt{\text{VOL}(R_a)}} \quad \text{if } i \in R_a \quad \text{and} \quad y_j := \frac{y'_b}{\sqrt{\text{VOL}(C_b)}} \quad \text{if } j \in C_b$$

with x'_a and y'_b that are coordinates of $\mathbf{x}' \in \mathbb{C}^k$ and $\mathbf{y}' \in \mathbb{C}^l$. Obviously, $\|\mathbf{D}_r^{1/2} \mathbf{x}\| = \|\mathbf{x}'\|$ and $\|\mathbf{D}_c^{1/2} \mathbf{y}\| = \|\mathbf{y}'\|$. Then, using $\bar{}$ for the complex conjugation,

$$\begin{aligned} |\langle \mathbf{x}, \mathbf{C} \mathbf{y} \rangle| &= \left| \sum_{i=1}^m \sum_{j=1}^n x_i \bar{y}_j c_{ij} \right| = \left| \sum_{a=1}^k \sum_{b=1}^l \frac{x'_a}{\sqrt{\text{VOL}(R_a)}} \frac{\bar{y}'_b}{\sqrt{\text{VOL}(C_b)}} c(R_a, C_b) \right| \\ &= \left| \sum_{a=1}^k \sum_{b=1}^l x'_a \bar{y}'_b c'_{ab} \right| = |\langle \mathbf{x}', \mathbf{C}' \mathbf{y}' \rangle| \leq s_{\max}(\mathbf{C}') \cdot \|\mathbf{x}'\| \cdot \|\mathbf{y}'\| \\ &= \|\mathbf{C}'\| \cdot \|\mathbf{D}_r^{1/2} \mathbf{x}\| \cdot \|\mathbf{D}_c^{1/2} \mathbf{y}\| \end{aligned}$$

by the well-known extremal property of the largest singular value, which finishes the proof.

Using this lemma and the starting steps of the proof of Theorem 1, with the matrix \mathbf{F} defined in (6) and the constructed step-vectors $\mathbf{x} \in \mathbb{C}^m$, $\mathbf{y} \in \mathbb{C}^n$, we have

$$s_k \leq \|\mathbf{D}_{\text{row}}^{-1/2} \mathbf{F} \mathbf{D}_{\text{col}}^{-1/2}\| \leq \frac{9}{2} |\langle \mathbf{x}, \mathbf{F} \mathbf{y} \rangle|.$$

We also know from [11] and the preliminary argument that \mathbf{x} takes on at most $r_1 = \Theta(\log m)$, and \mathbf{y} takes on at most $r_2 = \Theta(\log n)$ distinct values, which define the proper partitions P_1, \dots, P_{r_1} of the rows and Q_1, \dots, Q_{r_2} of the columns. Let us consider the subdivision of them with respect to R_1, \dots, R_k and C_1, \dots, C_k . In this way, we obtain the proper partition P'_1, \dots, P'_{ℓ_1} of the rows and Q'_1, \dots, Q'_{ℓ_2} of the columns with at most $\ell_1 = kr_1$ and $\ell_2 = kr_2$ parts.

Now, we apply Lemma 3 to the matrix \mathbf{F} and to the step-vectors \mathbf{x} and \mathbf{y} , which are also stepwise constant with respect to the above partitions. The row-weights and column-weights are the $d_{\text{row},i}$'s and $d_{\text{col},j}$'s, respectively. In view of the lemma, the entries of the $\ell_1 \times \ell_2$ matrix \mathbf{F}' are

$$f'_{ab} := \frac{f(P'_a, Q'_b)}{\sqrt{\text{Vol}(P'_a) \text{Vol}(Q'_b)}}$$

and

$$|\langle \mathbf{x}, \mathbf{F} \mathbf{y} \rangle| \leq \|\mathbf{F}'\| \cdot \|\mathbf{D}_{\text{row}}^{1/2} \mathbf{x}\| \|\mathbf{D}_{\text{col}}^{1/2} \mathbf{y}\| \leq \|\mathbf{F}'\|.$$

But by a well-known linear algebra fact,

$$\|\mathbf{F}'\| = s_{\max}(\mathbf{F}') \leq \sqrt{\ell_1 \ell_2} \max_{a \in \{1, \dots, \ell_1\}} \max_{b \in \{1, \dots, \ell_2\}} |f'_{ab}| \leq \ell \cdot \text{disc}_{R_1, \dots, R_k, C_1, \dots, C_k}(\mathbf{C}),$$

where $\ell = \sqrt{\ell_1 \ell_2}$ and we used Formula (2) for the discrepancy. Consequently,

$$s_k \leq \frac{9}{2} \ell \text{disc}_k(\mathbf{C})$$

follows. The drawback is that the upper bound contains $\ell = k\sqrt{r_1 r_2}$ which is of order $\sqrt{\log m \log n}$. Therefore, we prefer the estimate of Theorem 1 that does not contain the sizes of \mathbf{C} .

- Another dead-end was the attempt with the following matrix \mathbf{E} instead of \mathbf{F} of (6):

$$\mathbf{E} = \mathbf{C} - \mathbf{D}_{\text{row}} \hat{\mathbf{C}} \mathbf{D}_{\text{col}}, \quad (12)$$

where $\hat{\mathbf{C}} = \sum_{i=0}^{k-1} s_i \hat{\mathbf{v}}_i \hat{\mathbf{u}}_i^T$ is an $m \times n$ block-matrix of $k \times k$ blocks with entries equal to \hat{c}_{ab} over the block $R_a \times C_b$. The vectors $\hat{\mathbf{v}}_i \in \mathbb{R}^m$ and $\hat{\mathbf{u}}_i \in \mathbb{R}^n$ are stepwise constant over the partitions of R_1, \dots, R_k of the rows and C_1, \dots, C_k of the columns of \mathbf{C} , obtained by spectral clustering tools. The vectors $\hat{\mathbf{v}}_i$ and $\hat{\mathbf{u}}_i$ themselves were constructed via several SVDs in the proof of the forward statement of [10] so that $\mathbf{D}_{\text{row}}^{1/2} \hat{\mathbf{v}}_i$ and $\mathbf{D}_{\text{col}}^{1/2} \hat{\mathbf{u}}_i$ be ‘close’ to \mathbf{v}_i and \mathbf{u}_i , respectively, for $i = 1, \dots, k-1$ (for $i = 0$, they coincide), where $\mathbf{v}_i \in \mathbb{R}^m$, $\mathbf{u}_i \in \mathbb{R}^n$ is the unit-norm singular vector pair corresponding to s_i ($i = 1, \dots, r$). In particular, $\mathbf{v}_0 = (\sqrt{d_{\text{row},1}}, \dots, \sqrt{d_{\text{row},m}})^T$ and $\mathbf{u}_0 = (\sqrt{d_{\text{col},1}}, \dots, \sqrt{d_{\text{col},n}})^T$.

The point is that the so-called error matrix \mathbf{E} is close to the matrix $\mathbf{D}_{\text{row}}^{1/2}(\mathbf{C}_{\text{nor}} - \sum_{i=0}^{k-1} s_i \mathbf{v}_i \mathbf{u}_i^T) \mathbf{D}_{\text{col}}^{1/2}$, and $\|\mathbf{C}_{\text{nor}} - \sum_{i=0}^{k-1} s_i \mathbf{v}_i \mathbf{u}_i^T\| = s_k$. If now $\mathbf{x} \in \mathbb{C}^m$ and $\mathbf{y} \in \mathbb{C}^n$ are step-vectors such that $\|\mathbf{D}_{\text{row}}^{1/2} \mathbf{x}\| \leq 1$, $\|\mathbf{v}_k - \mathbf{D}_{\text{row}}^{1/2} \mathbf{x}\| \leq \frac{1}{3}$ and $\|\mathbf{D}_{\text{col}}^{1/2} \mathbf{y}\| \leq 1$, $\|\mathbf{u}_k - \mathbf{D}_{\text{col}}^{1/2} \mathbf{y}\| \leq \frac{1}{3}$, then,

$$s_k \leq \frac{9}{2} \langle (\mathbf{D}_{\text{row}}^{1/2} \mathbf{x}), (\mathbf{D}_{\text{row}}^{-1/2} \mathbf{C} \mathbf{D}_{\text{col}}^{-1/2} - \sum_{i=0}^{k-1} s_i \mathbf{v}_i \mathbf{u}_i^T) (\mathbf{D}_{\text{col}}^{1/2} \mathbf{y}) \rangle.$$

Here the upper bound is very close to $\frac{9}{2} |\langle \mathbf{x}, \mathbf{E} \mathbf{y} \rangle|$. The problem is that $\langle \mathbf{1}_X, \mathbf{E} \mathbf{1}_Y \rangle$ cannot be directly related to the discrepancy, like $\langle \mathbf{1}_X, \mathbf{F} \mathbf{1}_Y \rangle$. However, \mathbf{F} and \mathbf{E} are very ‘close’ to each other, since comparing Formulas (6) and (12), the difference between the corresponding entries of the block-matrices \mathbf{R} and $\hat{\mathbf{C}}$ is

$$|\rho(R_a, C_b) - \hat{c}_{ab}| = \frac{1}{\text{Vol}(R_a) \text{Vol}(C_b)} \left| \sum_{i \in R_a} \sum_{j \in C_b} \eta_{ij} \right|,$$

which is the density of the error matrix $\mathbf{E} = (\eta_{ij})$ between R_a and C_b . If this is small enough, we may expect a finer upper estimate for s_k , based on \mathbf{E} .

4 Conclusions and applications

4.1 Undirected graphs

The notion of multiway discrepancy naturally extends to edge-weighted graphs. A weighted undirected graph $G = (V, \mathbf{W})$ is uniquely characterized by its

weighted adjacency matrix \mathbf{W} , which is symmetric of nonnegative entries and zero diagonal. $\mathbf{D} = \text{diag}(d_1, \dots, d_n)$ is the diagonal *degree-matrix* ($d_i = \sum_{j=1}^n w_{ij}$), $\text{Vol}(U) = \sum_{i \in U} d_i$ is the volume of $U \subset V$, and for simplicity we assume that $\sum_{i=1}^n d_i = 1$; it does not hurt the generality, because neither the normalized matrix $\mathbf{W}_D = \mathbf{D}^{-1/2} \mathbf{W} \mathbf{D}^{-1/2}$, nor the multiway discrepancies to be introduced are affected by the scaling of \mathbf{W} . In case of a simple graph, \mathbf{W}_D is the *normalized adjacency matrix*. Definition 1 extends to this case as follows.

Definition 2 *The multiway discrepancy of the undirected, weighted graph $G = (V, \mathbf{W})$ in the proper k -partition V_1, \dots, V_k of its vertices is*

$$\text{disc}(G; V_1, \dots, V_k) = \max_{\substack{1 \leq a \leq b \leq k \\ X \subset V_a, Y \subset V_b}} \frac{|w(X, Y) - \rho(V_a, V_b) \text{Vol}(X) \text{Vol}(Y)|}{\sqrt{\text{Vol}(X) \text{Vol}(Y)}}.$$

The minimum k -way discrepancy of the undirected weighted graph $G = (V, \mathbf{W})$ is

$$\text{disc}_k(G) = \min_{V_1, \dots, V_k} \text{disc}(G; V_1, \dots, V_k).$$

A result, analogous to that of Theorem 1 can now be formulated in terms of the normalized modularity matrix of G , defined in [8] as follows. Denoting by $\mathbf{d} = (d_1, \dots, d_n)^T$ the *degree-vector* (of entries summing to 1), the so-called *modularity matrix* is $\mathbf{M} = \mathbf{W} - \mathbf{d}\mathbf{d}^T$, the (i, j) entry of which just measures the deviation of w_{ij} (actual connection of vertices i and j) from $d_i d_j$ (their connection under independent attachment with the vertex-degrees as probabilities). With the notation $\sqrt{\mathbf{d}} = (\sqrt{d_1}, \dots, \sqrt{d_n})^T$, the *normalized modularity matrix* is

$$\mathbf{M}_D = \mathbf{D}^{-1/2} \mathbf{M} \mathbf{D}^{-1/2} = \mathbf{W}_D - \sqrt{\mathbf{d}} \sqrt{\mathbf{d}}^T.$$

The spectrum of \mathbf{M}_D is in the $[-1, 1]$ interval, and 0 is always an eigenvalue with unit-norm eigenvector $\sqrt{\mathbf{d}}$. All the other eigenvalues are the same as those of \mathbf{W}_D , except the trivial one. Indeed, 1 is a single eigenvalue of \mathbf{W}_D with corresponding unit-norm eigenvector $\sqrt{\mathbf{d}}$, provided \mathbf{W} is irreducible. This becomes a zero eigenvalue of \mathbf{M}_D with the same eigenvector. In [9], I denoted the eigenvalues of \mathbf{M}_D in decreasing absolute values by $|\mu_1| \geq \dots \geq |\mu_{n-1}| \geq \mu_n = 0$. Then the absolute values of the eigenvalues of \mathbf{W}_D are $1 = \mu_0 \geq |\mu_1| \geq \dots \geq |\mu_{n-1}|$, and they are also the singular values: $s_k = |\mu_k|$, $k = 0, \dots, n-1$.

Proposition 1 *Let $G = (V, \mathbf{W})$ be an edge-weighted, undirected graph. Then*

$$|\mu_k| \leq 9 \text{disc}_k(G) (k + 2 - 9k \ln \text{disc}_k(G)), \quad (13)$$

where μ_k is the k -th largest absolute value eigenvalue of the normalized modularity matrix \mathbf{M}_D ($k = 1, \dots, n-1$).

Recall that Bilu and Linial [4] prove the following converse of the expander mixing lemma for d -regular simple graphs on n vertices. Assume that for any disjoint vertex-subsets S, T : $|e(S, T) - \frac{|S||T|d}{n}| \leq \alpha \sqrt{|S||T|}$. Then all but the largest adjacency eigenvalue of G are bounded (in absolute value) by $O(\alpha(1 + \log \frac{d}{\alpha}))$. Note that for a d -regular graph the adjacency eigenvalues are d times larger than the normalized adjacency ones, and the deviation between $e(S, T)$ and the one what is expected in a random d -regular graph, is also proportional

to our (1-way) discrepancy in terms of the volumes. Though they use disjoint subsets S, T , their upper estimate for the absolute value of the second largest (in absolute value) eigenvalue with the (1-way) discrepancy α is $C\alpha(1 - A \log \alpha)$ with some absolute constants A, C . Hence, the upper estimate of (4) or that of (13) in the $k = 1$ case are reminiscent of this.

In the other direction, for the $k = 1$ case, a straightforward generalization of the *expander mixing lemma for irregular graphs* is the following.

Proposition 2

$$\text{disc}(G) = \text{disc}_1(G) \leq \|\mathbf{M}_D\| = s_1 = |\mu_1|,$$

where $\|\mathbf{M}_D\|$ is the spectral norm of the normalized modularity matrix of G .

Though, with different notation (sometimes even a stronger version of it) is proved in [7, 13, 16], we give another short proof here.

Proof. Via separation theorems for singular values, $s_1 = |\mu_1|$ is the maximum of the bilinear form $\mathbf{v}^T \mathbf{M}_D \mathbf{u}$ over the unit sphere. Let $X, Y \subset V$ be arbitrary, and denote by $\mathbf{1}_X, \mathbf{1}_Y \in \mathbb{R}^n$ the indicator vectors of them. Then

$$\begin{aligned} \|\mathbf{M}_D\| &= \max_{\|\mathbf{u}\|=\|\mathbf{v}\|=1} |\mathbf{v}^T \mathbf{M}_D \mathbf{u}| \geq \left| \left(\frac{\mathbf{D}^{1/2} \mathbf{1}_X}{\|\mathbf{D}^{1/2} \mathbf{1}_X\|} \right)^T \mathbf{M}_D \left(\frac{\mathbf{D}^{1/2} \mathbf{1}_Y}{\|\mathbf{D}^{1/2} \mathbf{1}_Y\|} \right) \right| \\ &= \frac{|\mathbf{1}_X^T \mathbf{M}_D \mathbf{1}_Y|}{\|\mathbf{D}^{1/2} \mathbf{1}_X\| \cdot \|\mathbf{D}^{1/2} \mathbf{1}_Y\|} = \frac{|w(X, Y) - \text{Vol}(X)\text{Vol}(Y)|}{\sqrt{\text{Vol}(X)}\sqrt{\text{Vol}(Y)}}. \end{aligned}$$

Taking the maxima on the right-hand side over subsets $X, Y \subset V$, the desired relation follows. Note that the estimate is also valid if we take maxima over disjoint X, Y pairs only.

For an arbitrary k (between 1 and $\text{rank} \mathbf{W}$), in Theorem 3 of [9] we proved that under some balancing conditions for the degrees and the cluster sizes (when $n \rightarrow \infty$), and denoting by V_1, \dots, V_k the clusters obtained by spectral clustering (see the forthcoming explanation), the (V_a, V_b) pairs are $O(\sqrt{2k}S_k + |\mu_k|)$ -volume regular ($a \neq b$) and similar statement holds for the subgraphs induced by V_a 's too. In fact, inspired by [3], there we used a bit different notation and concept of α -volume regular pairs, namely, for every $X \subseteq V_a, Y \subseteq V_b$ we required

$$|w(X, Y) - \rho(V_a, V_b)\text{Vol}(X)\text{Vol}(Y)| \leq \alpha \sqrt{\text{Vol}(V_a)\text{Vol}(V_b)}.$$

In the above formula, the right hand side contains the squareroots of the volumes of the clusters, unlike (3), which contains the squareroots of the volumes of X and Y . However, in the spirit of the Szemerédi regularity lemma [26], if we require (3) to hold only for X, Y 's satisfying $\text{Vol}(X) \geq \varepsilon \text{Vol}(V_i)$, $\text{Vol}(Y) \geq \varepsilon \text{Vol}(V_j)$ with some fixed ε , then the so modified k -way discrepancy, $\text{disc}'_k(G)$, is $O(\sqrt{2k}S_k + |\mu_k|)$, and so does $\text{disc}_k(G)$. Here the partition V_1, \dots, V_k is defined so that it minimizes the weighted k -variance S_k^2 of the vertex representatives $\mathbf{r}_1, \dots, \mathbf{r}_n \in \mathbb{R}^{k-1}$ obtained as row vectors of the $n \times (k-1)$ matrix of column vectors $\mathbf{D}^{-1/2} \mathbf{u}_i$, where \mathbf{u}_i is the unit-norm eigenvector corresponding to μ_i ($i = 1, \dots, k-1$). The k -variance of the representatives is defined as

$$S_k^2(\mathbf{X}) = \min_{(V_1, \dots, V_k)} \sum_{a=1}^k \sum_{j \in V_a} d_j \|\mathbf{r}_j - \mathbf{c}_a\|^2, \quad (14)$$

where $\mathbf{c}_a = \frac{1}{\text{vol}(V_a)} \sum_{j \in V_a} d_j \mathbf{r}_j$ is the weighted center of cluster V_a . It is the weighted k -means algorithm that gives this minimum, and the point is that the optimum S_k is just the minimum distance between the eigensubspace corresponding to μ_0, \dots, μ_{k-1} and the one of the suitably transformed step-vectors over the k -partitions of V . In [9] we also discussed that, in view of subspace perturbation theorems, the larger the gap between $|\mu_{k-1}|$ and $|\mu_k|$, the smaller S_k is. So the message is, that here the eigenvectors corresponding to the largest absolute value eigenvalues have to be used, unlike usual spectral clustering methods which automatically use the bottom eigenvalues of the Laplacian or normalized Laplacian matrix (latter one is just $\mathbf{I} - \mathbf{W}_D$). The clusters or cluster-pairs of small discrepancy behave like expanders or bipartite expanders. In another context, they resemble the generalized random or quasirandom graphs of Lovász, Sós, Simonovits [23, 24].

In some special cases, $S_k = 0$, and then, $\text{disc}_k(G) \leq B|\mu_k| = Bs_k$ follows from the above results. In particular, $S_k = 0$ whenever the vectors $\mathbf{D}^{-1/2}\mathbf{u}_1, \dots, \mathbf{D}^{-1/2}\mathbf{u}_{k-1}$ are step-vectors over the same proper k -partition of the vertices. Some examples:

- If $k = 1$, then the unit-norm eigenvector corresponding to $\mu_0 = 1$ is $\mathbf{u}_0 = \sqrt{\mathbf{d}}$, and $\mathbf{D}^{-1/2}\mathbf{u}_0 = \mathbf{1}$ is the all 1's vector. Consequently, the variance of its coordinates is $S_1 = 0$. But in this case, by Proposition 2, we already know that $\text{disc}(G)$ can be estimated from above merely by $|\mu_1| = s_1$.
- If $k = 2$ and G is bipartite, then $\mu_1 = -1$, $s_1 = 1$, and S_2^2 , i.e., the 2-variance of the coordinates of the transformed eigenvector corresponding to μ_1 can be small if $|\mu_2|$ is separated from $|\mu_1| = 1$ (see also the bipartite expanders of [1]).
- Let $k = 2$ and G be bipartite, biregular on the independent vertex-subsets V_1, V_2 . That is, all the edge-weights within V_1 or V_2 are zeros, and the 0-1 weights between vertices of V_1 and V_2 are such that $d_i = k_1$ if $i \in V_1$ and $d_i = k_2$ if $i \in V_2$ with the understanding that $|V_1|k_1 = |V_2|k_2$ (both are the total number of edges in G). It is easy to see that the unit-norm eigenvector corresponding to the eigenvalue $\mu_1 = -1$ is $\mathbf{u}_1 = \mathbf{D}^{1/2}\mathbf{1}_{V_1} - \mathbf{D}^{1/2}\mathbf{1}_{V_2}$, and $\mathbf{D}^{-1/2}\mathbf{u}_1 = \mathbf{1}_{V_1} - \mathbf{1}_{V_2}$. Therefore, the representatives of vertices of V_1 are all 1's, and those of V_2 are -1 's, so $S_2 = 0$. Consequently, $\text{disc}_2(G) \leq B|\mu_2|$, with some absolute constant B . Up to a constant, this was another proof of Lemma 3.2 of Evra et al. [18]. They call their result expander mixing lemma for bipartite graphs, and use cardinalities instead of volumes, but in this special case, these cardinalities are proportional to the volumes both within V_1 and V_2 .
- Let G_n be a generalized random graph over the symmetric $k \times k$ pattern matrix $\mathbf{P} = (p_{ab})$, i.e., there is a proper k -partition, V_1, \dots, V_k , of its vertices such that $|V_a| = n_a$ ($a = 1, \dots, k$), $\sum_{a=1}^k n_a = n$, and for any $1 \leq a \leq b \leq k$, vertices $i \in V_a$ and $j \in V_b$ are connected independently, with the same probability p_{ab} . This is the k -cluster generalization of the classical Erdős–Rényi random graph, see also [23] for their generalized quasirandom counterparts. In [6] we characterized the adjacency and

normalized Laplacian spectra of such graphs, that extends to their normalized modularity spectra as follows: both $|\mu_k| = s_k$ and S_k tend to zero almost surely when $n \rightarrow \infty$, under some balancing conditions for the cluster sizes ($\frac{n_a}{n} \geq c$ with some constant c , for $a = 1, \dots, k$). By our results, it also holds for the k -way discrepancy in the clustering V_1, \dots, V_k . However, this is not surprising, since this almost sure limit for the k -way discrepancy is easily obtained with large deviation principles too, see [5].

Summarizing, in the $k = 1$ case: when the second singular value $|\mu_1| = s_1$ is small (much smaller than $s_0 = 1$), then the overall discrepancy is small. But for $k > 1$, a small s_k is necessary, but not sufficient for a small k -way discrepancy. In addition, S_k should be small too. With subspace perturbation theorems, it is small if s_k is much smaller than s_{k-1} . Hence, a gap in the normalized modularity spectrum may be an indication for the number of clusters. The two directions together may give a hint about the optimal choice of k if a practitioner wants to find a k -clustering of the rows and columns (or just of the vertices of a graph) with small pairwise discrepancies. If there not exists a fairly ‘small’ k with this property, then in the worst case scenario, the Szemerédi regularity lemma [26] with an enormously large number of clusters (which number only depends on the maximum pairwise discrepancy to be attained, and does not depend on n) comes into existence. Weak versions of this lemma (where V_1, \dots, V_k are not necessarily equitable) are also available, see e.g., [12, 22].

Note that \mathbf{M}_D corresponds to the compact operator taking conditional expectation between the margins with respect to the symmetric joint distribution embodied by \mathbf{W} . In [9] we proved that for given k , the eigenvalues μ_1, \dots, μ_{k-1} and the corresponding eigensubspace are testable, consequently S_k is also testable, in the sense of [12]. This is important when we have a very large network and want to estimate these quantities based on a smaller sample selected with an appropriate randomization from the large one. We also remark that spectral or operator proofs of the regularity lemma, together with low-rank constructions, are at our disposal, for example, [19, 20, 25].

4.2 Directed graphs

A directed weighted graph $G = (V, \mathbf{W})$ is described by its quadratic, but usually not symmetric weight matrix $\mathbf{W} = (w_{ij})$ of zero diagonal, where w_{ij} is the nonnegative weight of the $i \rightarrow j$ edge ($i \neq j$). The row-sums $d_{out,i} = \sum_{j=1}^n w_{ij}$ and column-sums $d_{in,j} = \sum_{i=1}^n w_{ij}$ of \mathbf{W} are the out- and in-degrees, while $\mathbf{D}_{out} = \text{diag}(d_{out,1}, \dots, d_{out,n})$ and $\mathbf{D}_{in} = \text{diag}(d_{in,1}, \dots, d_{in,n})$ are the diagonal out- and in-degree matrices, respectively. Now Definition 1 can be formulated as follows.

Definition 3 *The multiway discrepancy of the directed, weighted graph $G = (V, \mathbf{W})$ in the in-clustering $V_{in,1}, \dots, V_{in,k}$ and out-clustering $V_{out,1}, \dots, V_{out,k}$ of its vertices is*

$$\begin{aligned} & \text{disc}(G; V_{in,1}, \dots, V_{in,k}, V_{out,1}, \dots, V_{out,k}) \\ &= \max_{\substack{1 \leq a \leq b \leq k \\ X \subset V_{out,a}, Y \subset V_{in,b}}} \frac{|w(X, Y) - \rho(V_{out,a}, V_{in,b}) \text{Vol}_{out}(X) \text{Vol}_{in}(Y)|}{\sqrt{\text{Vol}_{out}(X) \text{Vol}_{in}(Y)}}, \end{aligned}$$

where $w(X, Y)$ is the sum of the weights of the $X \rightarrow Y$ edges, whereas $\text{Vol}_{\text{out}}(X) = \sum_{i \in X} d_{\text{out},i}$ and $\text{Vol}_{\text{in}}(Y) = \sum_{j \in Y} d_{\text{in},j}$ are the out- and in-volumes, respectively. The minimum k -way discrepancy of the directed weighted graph $G = (V, \mathbf{W})$ is

$$\text{disc}_k(G) = \min_{\substack{V_{\text{in},1}, \dots, V_{\text{in},k} \\ V_{\text{out},1}, \dots, V_{\text{out},k}}} \text{disc}(G; V_{\text{in},1}, \dots, V_{\text{in},k}, V_{\text{out},1}, \dots, V_{\text{out},k}).$$

Butler [13] treats the $k = 1$ case, and for a general k , Theorem 1 implies the following.

Proposition 3 *Let $G = (V, \mathbf{W})$ be directed edge-weighted graph. Then*

$$s_k \leq 9 \text{disc}_k(G)(k + 2 - 9k \ln \text{disc}_k(G)),$$

where s_k is the k -th largest nontrivial singular value of the normalized edge-weight matrix $\mathbf{W}_D = \mathbf{D}_{\text{out}}^{-1/2} \mathbf{W} \mathbf{D}_{\text{in}}^{-1/2}$.

We applied the SVD based algorithm to find migration patterns in the set of 75 countries, and found 3 underlying immigration and emigrationin trait clusters. Since the algorithm is the same as for rectangular matrices, I will describe it in the next subsection.

4.3 Back to rectangular arrays

In multivariate statistics, sometimes our data are collected in an $m \times n$ matrix \mathbf{C} , where the entries are frequency counts corresponding to the joint distribution of two categorized random variables (taking on m and n discrete values, respectively). Such a \mathbf{C} is called contingency table in statistical language, and the data are popularly said to be cross-tabulated. The χ^2 statistic, which measures the deviation from independence, is $N \sum_{i=1}^{r-1} s_i^2$ with my notation, where N is the (usually ‘large’) sample size, but the second factor can be ‘small’ if s_1 is ‘small’, and this corresponds to the existence of a good rank 1 approximation of \mathbf{C} . This fact is also supported by the $\text{disc}(\mathbf{C}) = \text{disc}_1(\mathbf{C}) \leq s_1$ relation. Otherwise, one may ask, whether there exists a ‘good’ rank k approximation for some integer $1 < k < r = \text{rank}(\mathbf{C})$, which problem is treated in correspondence analysis by the first k dyads of the SVD of \mathbf{C}_D . However, there it is not made exact how s_k is estimated by $\text{disc}_k(\mathbf{C})$. Our Theorem 1 says that if the minimum k -way discrepancy is very ‘small’, i.e., the sub-tables $R_a \times C_b$ behave like independent tables in the optimal k -partitions of the rows and columns, then s_k is small too.

In the other direction, in [10], we proved the following. Given the $m \times n$ contingency table \mathbf{C} , consider the spectral clusters R_1, \dots, R_k of its rows and C_1, \dots, C_k of its columns, obtained by applying the k -means algorithm for the $(k - 1)$ -dimensional row- and column representatives, defined as the row vectors of the matrices of column vectors $(\mathbf{D}_{\text{row}}^{-1/2} \mathbf{v}_1, \dots, \mathbf{D}_{\text{row}}^{-1/2} \mathbf{v}_{k-1})$ and $(\mathbf{D}_{\text{col}}^{-1/2} \mathbf{u}_1, \dots, \mathbf{D}_{\text{col}}^{-1/2} \mathbf{u}_{k-1})$, respectively, where $\mathbf{v}_i, \mathbf{u}_i$ is the unit norm singular vector pair corresponding to s_i ($i = 1, \dots, k - 1$). In fact, these partitions minimize the weighted k -variances $S_{k,\text{row}}^2$ and $S_{k,\text{col}}^2$ of these row- and column-representatives (see (14)). Then, under some balancing conditions for the margins and for the cluster sizes, we proved that $\text{disc}_k(\mathbf{C}) \leq B(\sqrt{2k}(S_{k,\text{row}} +$

$S_{k,col}) + s_k)$, with some absolute constant B . This is the base of our algorithm, with fixed k .

We remark that the correspondence analysis uses the above $(k-1)$ -dimensional row- and column-representatives for simultaneously plotting the row- and column-categories in \mathbb{R}^{k-1} ($k = 2, 3$ or 4 in most applications), and hence, the practitioner can draw conclusions from their mutual positions. For example, in microarray analysis we can plot the genes and conditions together, and the biclusters obtained by k -clustering the row- and column-representatives give clusters of the genes and the conditions such that, every gene-cluster and condition-cluster pair behaves like a random weighted bipartite graph in the sense, that genes and conditions of the same cluster nearly independently influence each other, which fact may have importance for practitioners. In [10] it is also shown that when these k -variances are very ‘small’, then our construction (described there with the modified dyads) for the rank k approximation produces a table of nonnegative entries. On the contrary, a drawback of correspondence analysis is that the automatic low-rank approximation of the table usually contains negative entries.

In the possession of networks or microarrays, practitioners want to find a fairly small k , such that there is a k -cluster structure behind the table or the graph in the sense that the subgraphs and bipartite subgraphs have ‘small’ discrepancy. It depends on the table or the graph that how small discrepancy can be attained and with what k . The above theory tells that we have to inspect the normalized spectra, together with spectral subspaces, since the leading ones carry a lot of information about the smallest attainable discrepancy.

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